



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:34 PM JST

PDB ID : 7WED
EMDB ID : EMD-32447
Title : SARS-CoV-2 Omicron variant spike RBD in complex with Fab XGv347
Authors : Wang, X.; Wang, L.
Deposited on : 2021-12-23
Resolution : 3.50 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3358 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	201	1610	1038	273	291	8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	LEU	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	496	SER	GLY	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 2 is a protein called The heavy chain of Fab XGv347.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	123	941	588	158	189	6	0	0

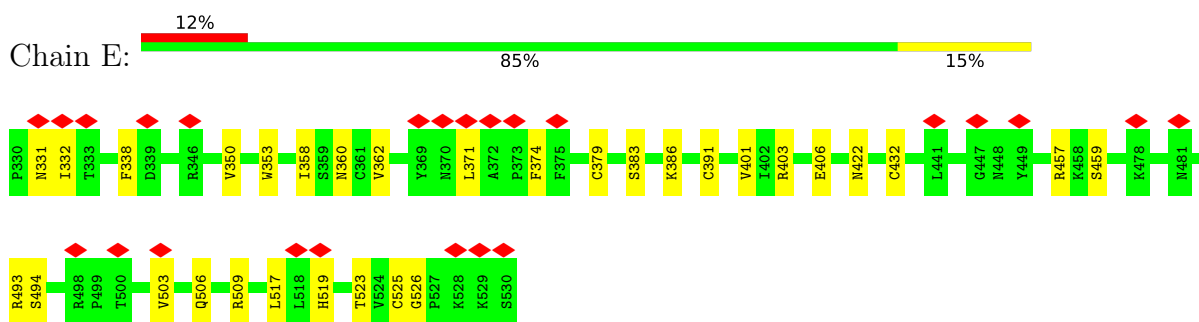
- Molecule 3 is a protein called The light chain of Fab XGv347.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	107	807	506	141	158	2	0	0

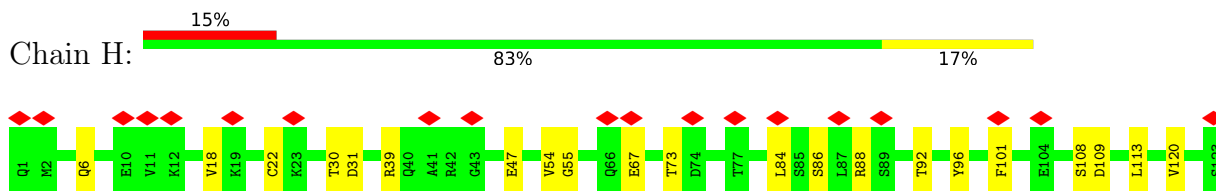
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

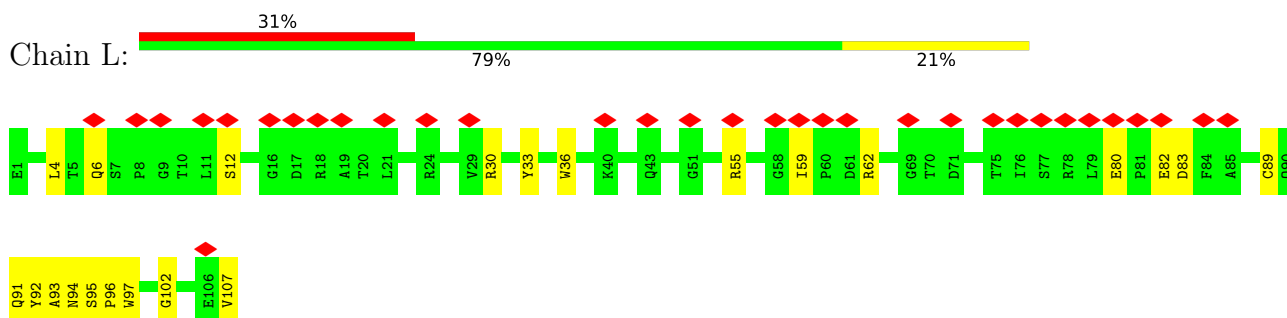
- Molecule 1: Spike protein S1



- Molecule 2: The heavy chain of Fab XGv347



- Molecule 3: The light chain of Fab XGv347



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.343	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0463	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.26	0/1658	0.52	0/2255
2	H	0.25	0/961	0.56	0/1306
3	L	0.27	0/826	0.55	0/1125
All	All	0.26	0/3445	0.54	0/4686

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1610	0	1548	21	0
2	H	941	0	903	14	0
3	L	807	0	779	12	0
All	All	3358	0	3230	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:CYS:HA	1:E:432:CYS:HB2	1.50	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:CYS:HA	1:E:525:CYS:HB3	1.57	0.86
3:L:95:SER:HB3	3:L:96:PRO:HD2	1.77	0.67
2:H:86:SER:O	2:H:88:ARG:NH1	2.30	0.64
1:E:362:VAL:HG13	1:E:526:GLY:HA2	1.79	0.64
1:E:457:ARG:NH1	1:E:459:SER:O	2.32	0.63
3:L:36:TRP:NE1	3:L:89:CYS:SG	2.72	0.62
1:E:379:CYS:HA	1:E:432:CYS:CB	2.29	0.61
1:E:403:ARG:HB2	1:E:406:GLU:HG3	1.86	0.57
1:E:493:ARG:NH2	2:H:55:GLY:O	2.38	0.57
1:E:331:ASN:HB2	1:E:332:ILE:HA	1.87	0.55
1:E:517:LEU:O	1:E:519:HIS:ND1	2.41	0.54
3:L:62:ARG:NH1	3:L:83:ASP:OD1	2.40	0.54
3:L:92:TYR:O	3:L:97:TRP:NE1	2.41	0.53
3:L:4:LEU:HD11	3:L:91:GLN:HG3	1.91	0.52
2:H:92:THR:HA	2:H:120:VAL:O	2.10	0.52
2:H:101:PHE:CE1	2:H:113:LEU:HD21	2.45	0.51
2:H:18:VAL:HG12	2:H:84:LEU:HB3	1.94	0.50
1:E:338:PHE:HE1	1:E:358:ILE:HD13	1.75	0.50
2:H:109:ASP:OD2	2:H:109:ASP:N	2.45	0.50
2:H:6:GLN:HG2	2:H:22:CYS:HB3	1.94	0.49
2:H:6:GLN:HE22	2:H:96:TYR:HA	1.79	0.48
1:E:371:LEU:HD23	1:E:374:PHE:HE2	1.79	0.47
1:E:371:LEU:HB3	1:E:374:PHE:CE2	2.49	0.47
3:L:6:GLN:OE1	3:L:102:GLY:N	2.40	0.47
2:H:30:THR:HG22	2:H:31:ASP:H	1.79	0.47
2:H:108:SER:OG	2:H:109:ASP:N	2.48	0.47
2:H:30:THR:HG22	2:H:31:ASP:N	2.30	0.47
1:E:391:CYS:HA	1:E:525:CYS:CB	2.36	0.46
1:E:360:ASN:H	1:E:523:THR:HG22	1.81	0.45
3:L:55:ARG:NH2	3:L:59:ILE:O	2.35	0.45
3:L:33:TYR:HD2	3:L:93:ALA:HB2	1.82	0.44
3:L:94:ASN:CG	3:L:95:SER:H	2.21	0.44
1:E:350:VAL:HG12	1:E:422:ASN:HB3	2.00	0.44
1:E:503:VAL:HG13	1:E:506:GLN:HE22	1.83	0.44
3:L:80:GLU:OE1	3:L:82:GLU:HG2	2.19	0.43
1:E:503:VAL:HA	1:E:506:GLN:HE22	1.83	0.43
1:E:383:SER:HB3	1:E:386:LYS:HD3	2.02	0.42
2:H:54:VAL:HG12	2:H:73:THR:HG21	2.01	0.42
1:E:493:ARG:HG2	1:E:494:SER:H	1.85	0.42
2:H:39:ARG:NE	2:H:47:GLU:OE1	2.45	0.42
1:E:401:VAL:HG22	1:E:509:ARG:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:30:ARG:HD2	3:L:30:ARG:HA	1.89	0.41
2:H:67:GLU:OE1	2:H:67:GLU:N	2.55	0.40
3:L:12:SER:OG	3:L:107:VAL:O	2.29	0.40
1:E:350:VAL:O	1:E:353:TRP:HD1	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
2	H	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
3	L	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	425/431 (99%)	390 (92%)	35 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	175/175 (100%)	175 (100%)	0	100	100
2	H	105/106 (99%)	105 (100%)	0	100	100
3	L	87/90 (97%)	87 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	367/371 (99%)	367 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

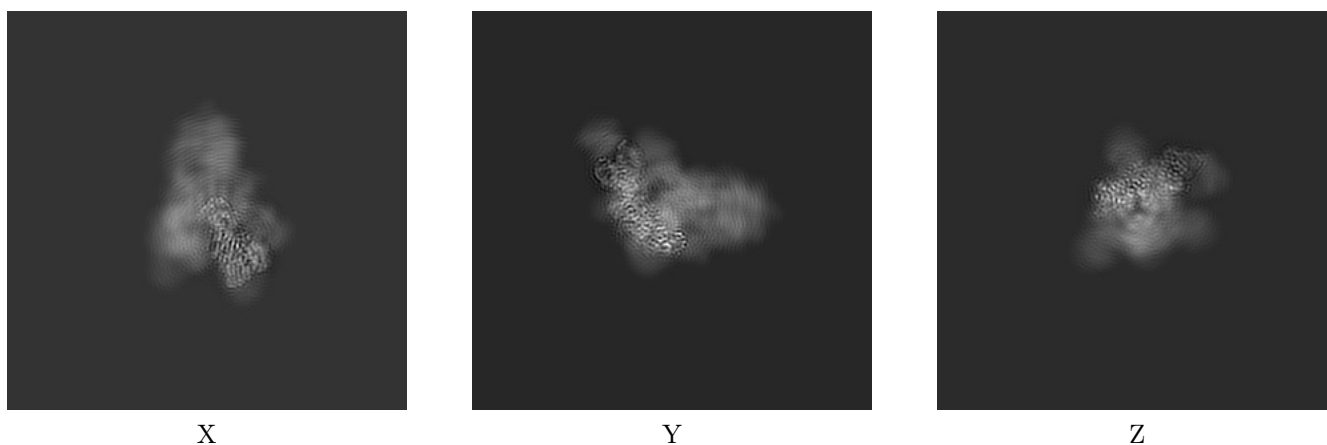
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32447. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

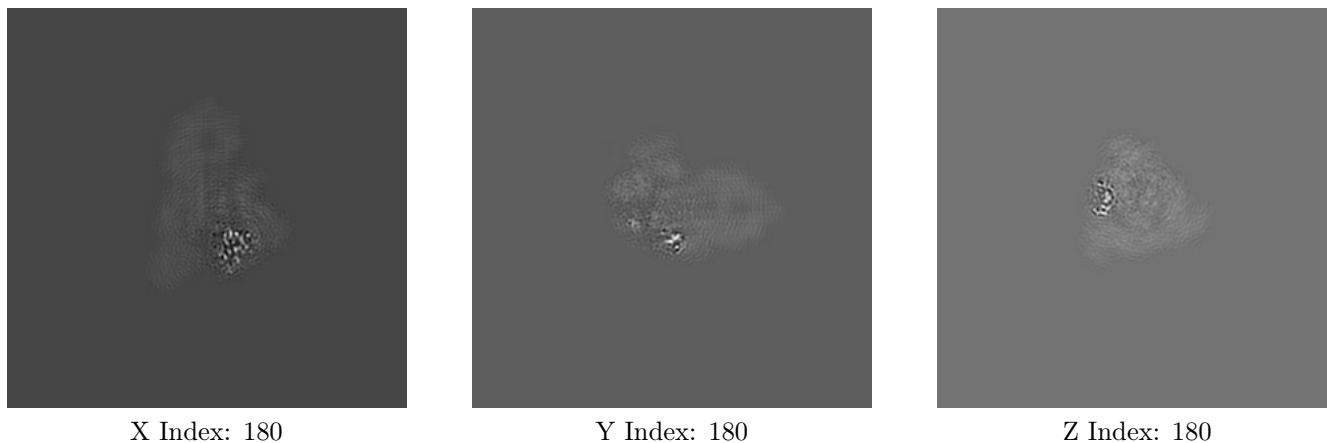
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

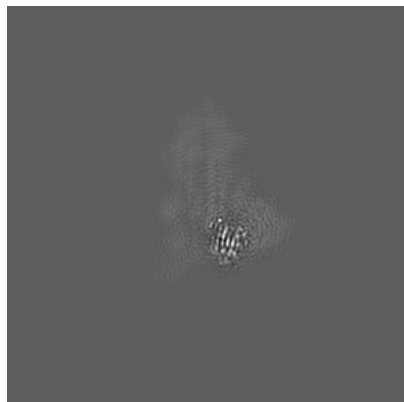
6.2.1 Primary map



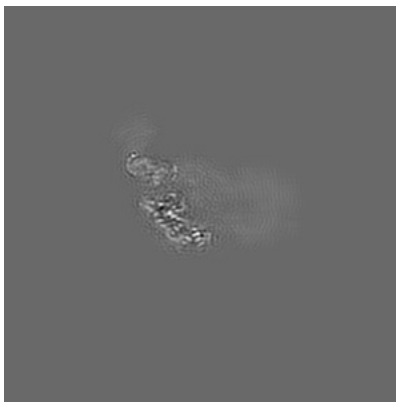
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

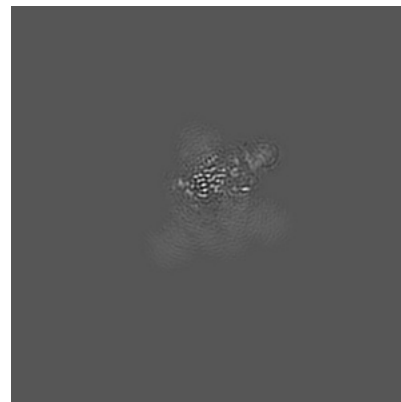
6.3.1 Primary map



X Index: 172



Y Index: 199



Z Index: 148

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0463. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

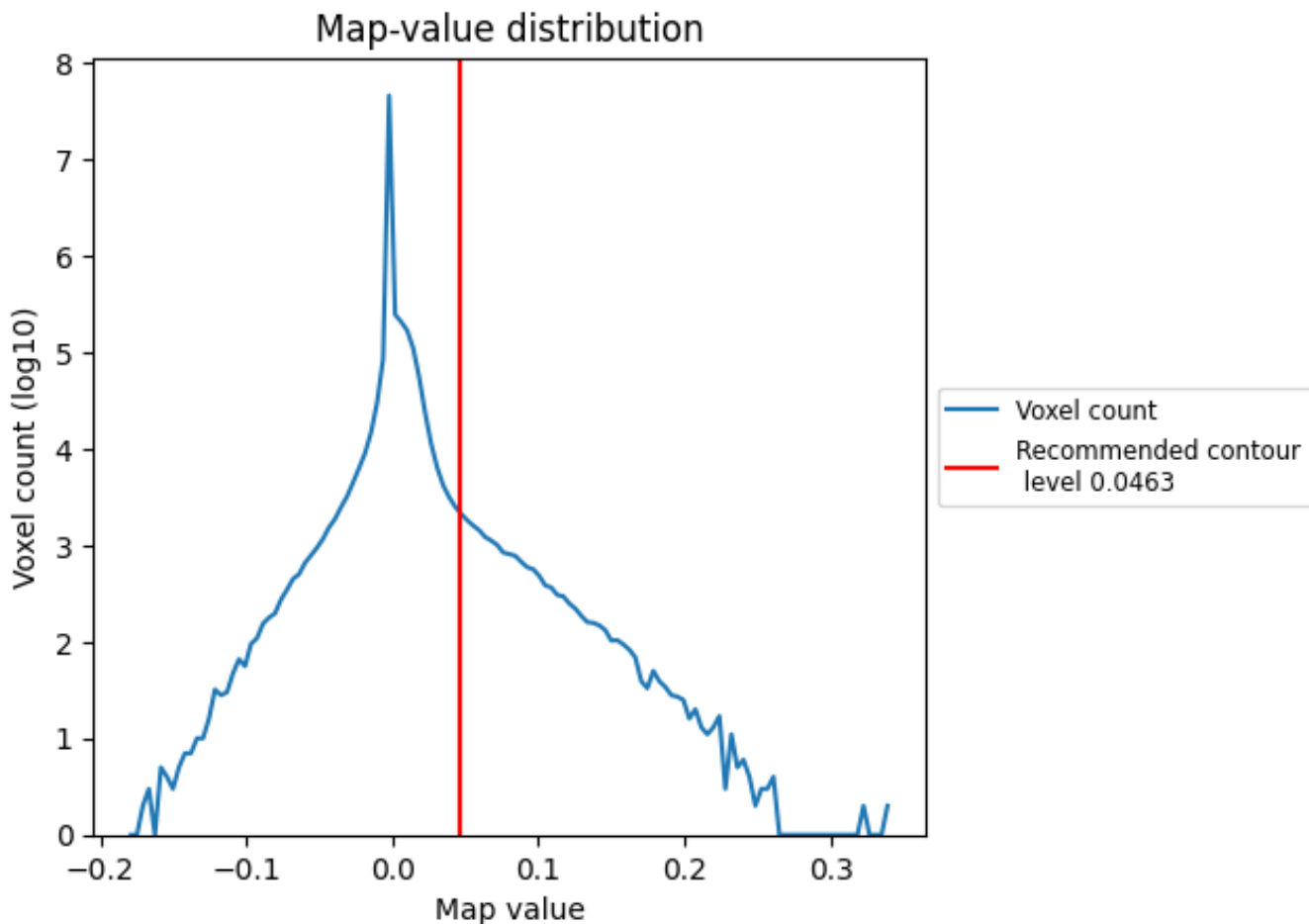
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

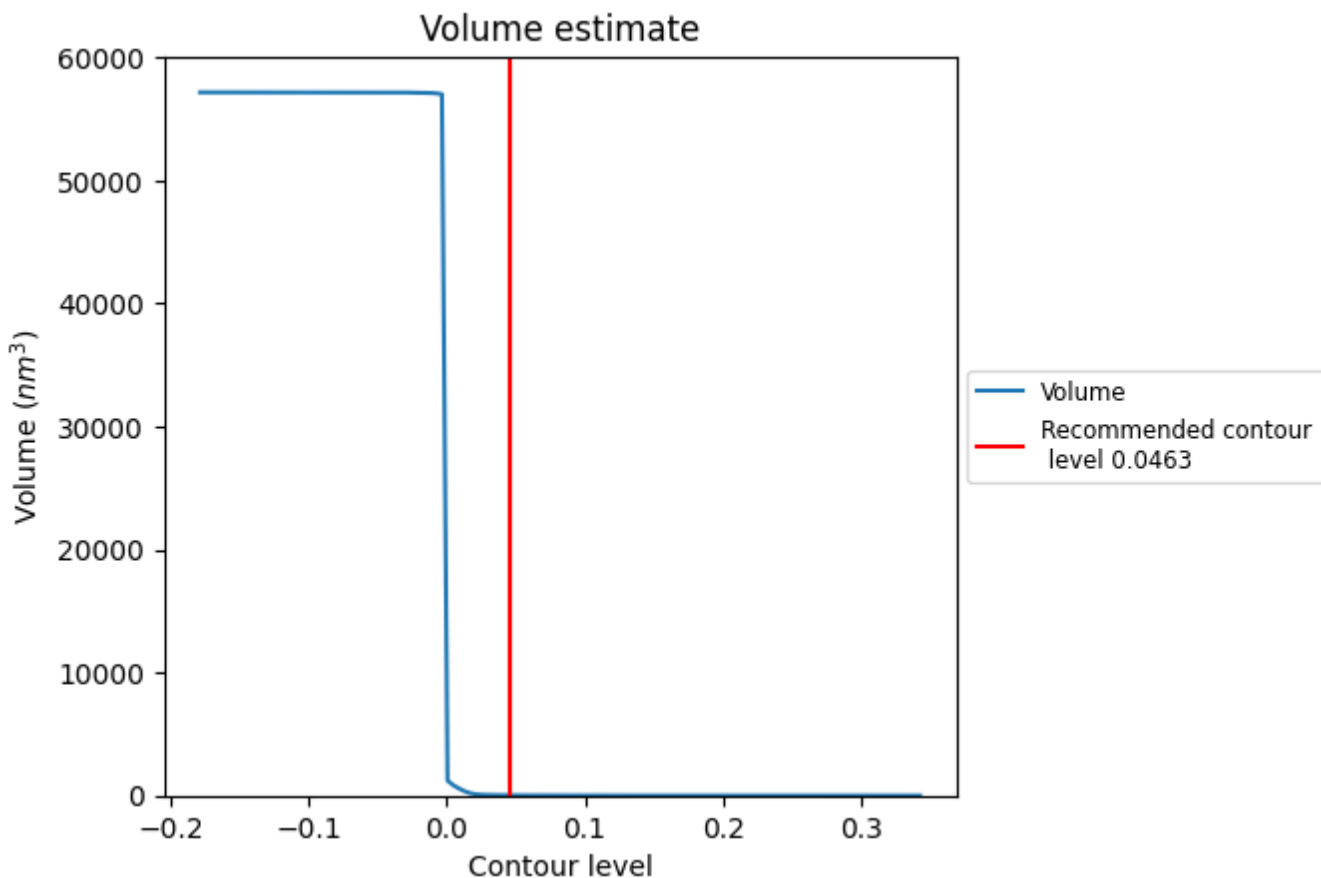
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

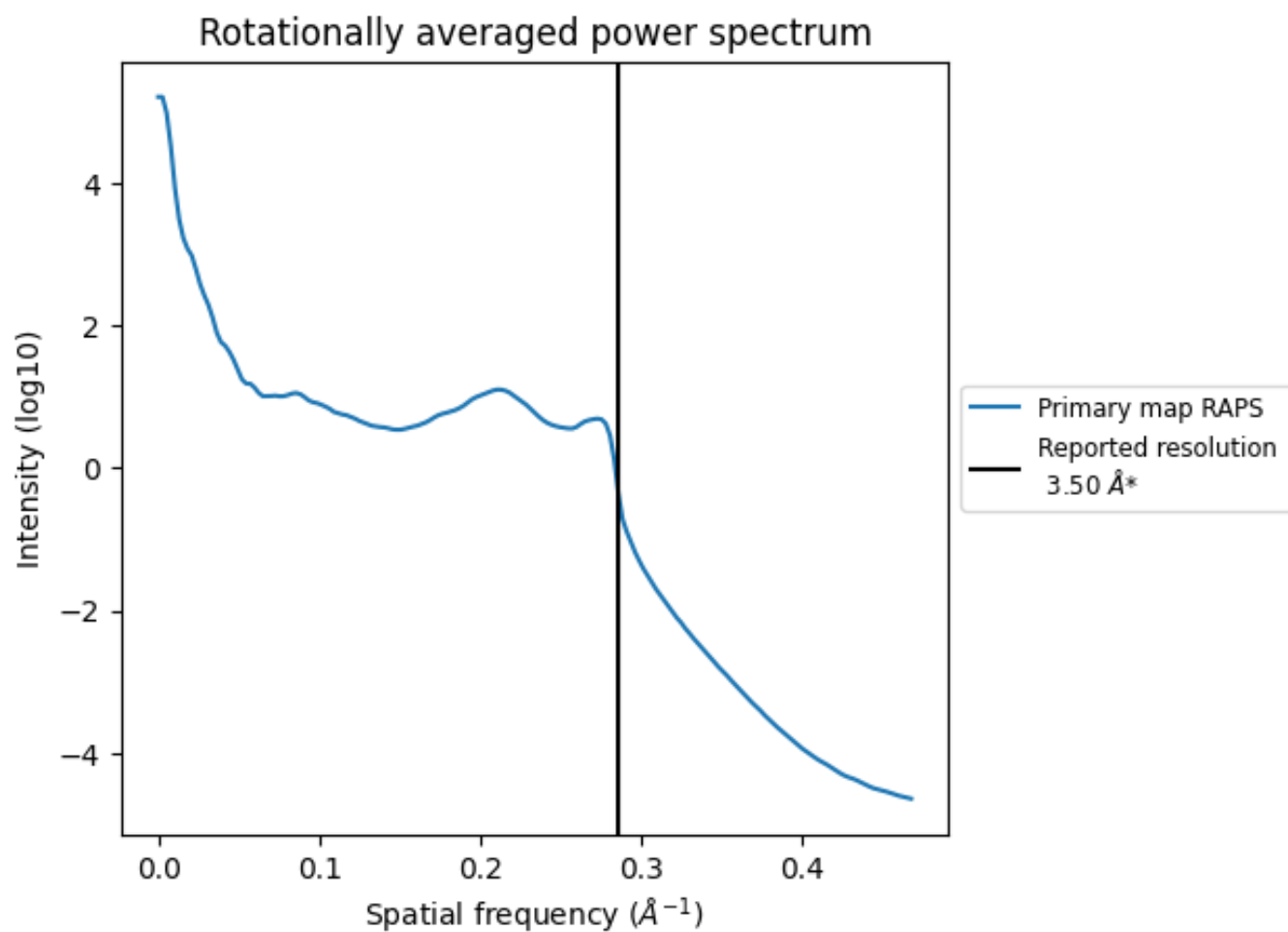
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm³; this corresponds to an approximate mass of 21 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286\AA^{-1}

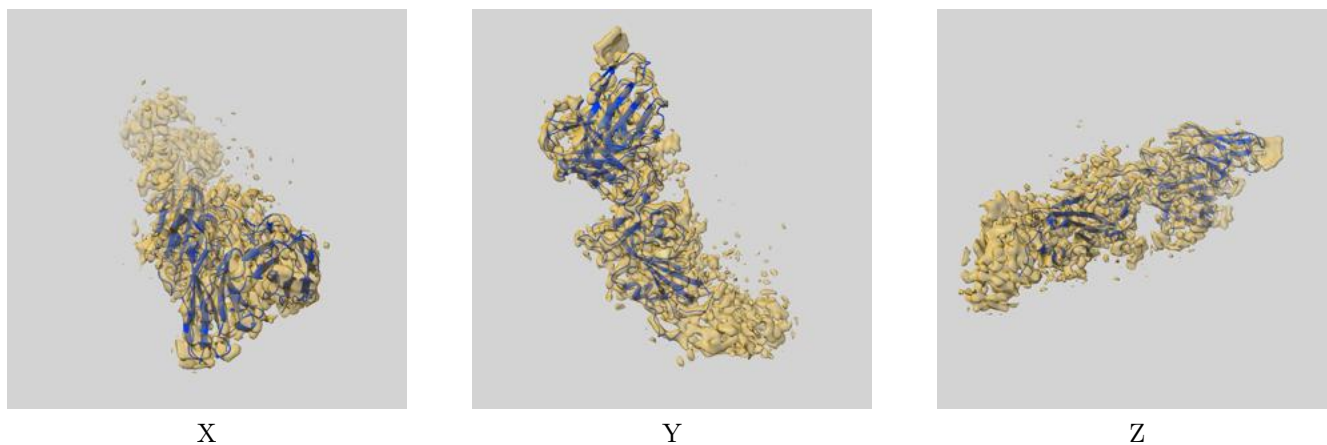
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

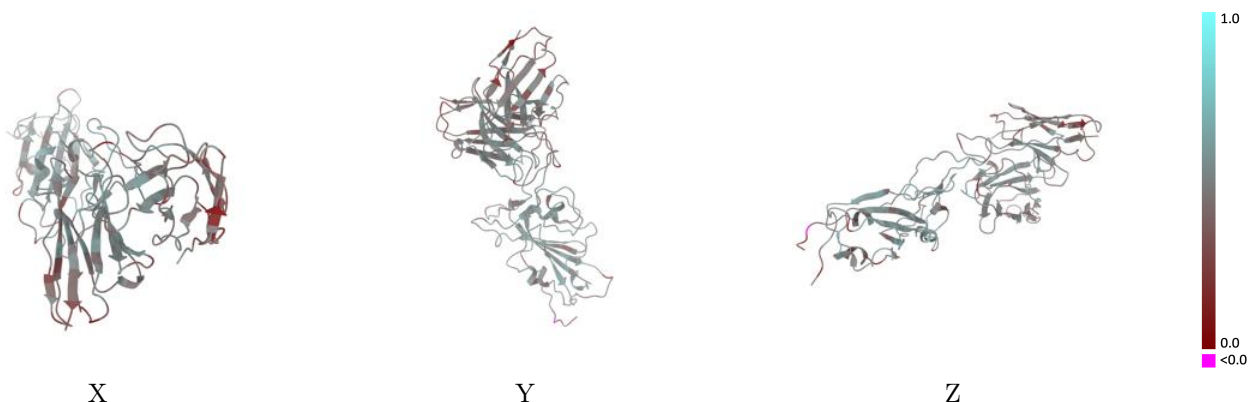
This section contains information regarding the fit between EMDB map EMD-32447 and PDB model 7WED. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



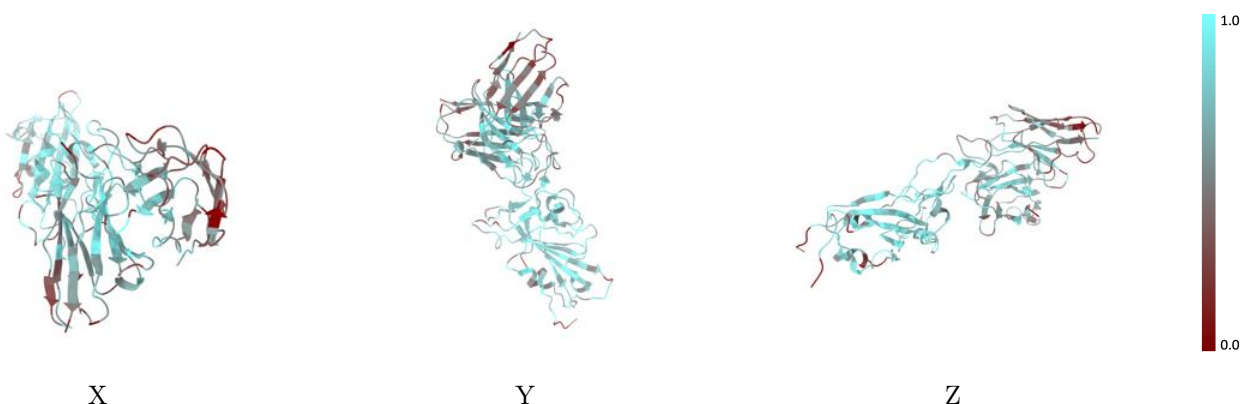
The images above show the 3D surface view of the map at the recommended contour level 0.0463 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



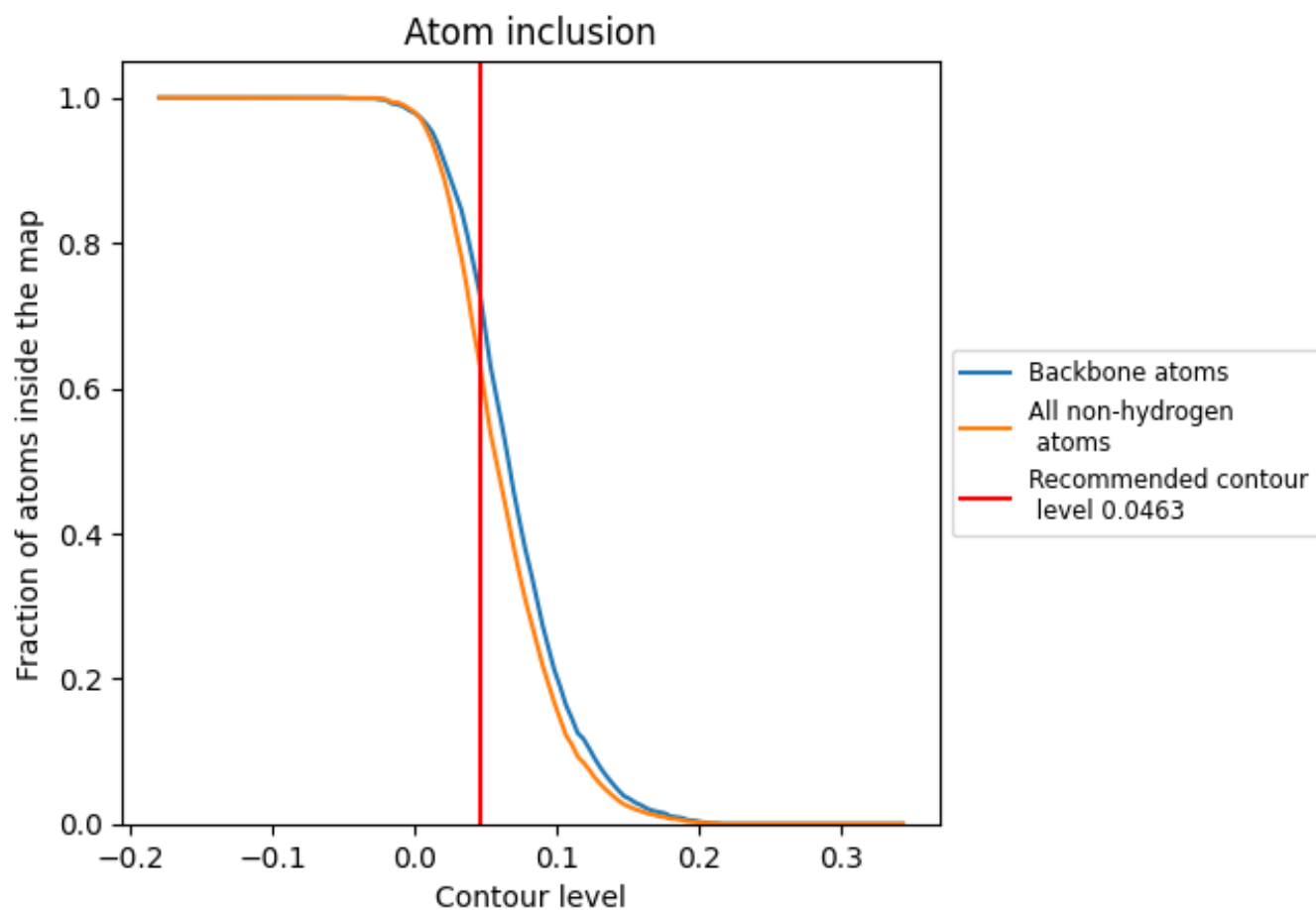
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0463).









9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0463) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6302	 0.4670
E	 0.6919	 0.4860
H	 0.6121	 0.4580
L	 0.5280	 0.4390

